Ecosystem Predictions with Approximate vs. Exact Light Fields

FINAL REPORT

On Work Performed by

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Ten-year simulations were performed using a coupled physical-biological-optical ocean ecosystem model with both simple analytic and accurate EcoLight numerical computations of the in-water irradiances. The predicted chlorophyll concentrations differed by tens of percent over the course of 10-year simulations. The EcoLight code runs with less than a 30% increase in run time, while providing several advantages than cannot be obtained with an analytic light model. These advantages are as follows. (1) EcoLight does a much better job of computing irradiances near 400 and beyond 600 nm, and at depth. These differences can have significant effects on how particular phytoplankton functional groups evolve in time and at depth. (2) EcoLight can model any water body, including Case 2 water and optically shallow waters for which bottom reflectance can substantially increase the irradiance available for photosynthesis and water heating. (3) EcoLight provides the outputs necessary for ecosystem validation using satellite-derived water-leaving radiances or remote-sensing reflectances, without the necessity of using a chlorophyll algorithm to convert satellite data into an ecosystem variable. (4) EcoLight provides a means for improved ecosystem model initialization and data assimilation directly in terms of the available data, again without an intermediate step involving a data-to-chlorophyll conversion algorithm.

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1. Executive Summary

Coupled physical-biological-optical ecosystem models often use sophisticated treatments of their physical and biological components, while oversimplifying the optical component to the detriment of the ecosystem predictions. To bring optical computations up to the standard required by recent ecosystem models, I previously developed (as a part of the Hyperspectral Coastal Ocean Dynamics Experiment (HyCODE) under ONR contract N00014-05-M-0146) a computationally fast numerical model named EcoLight, derived from the HydroLight numerical model, which computes accurate in-water irradiances for use in biological primary production calculations. In the present work, my colleagues and I incorporated EcoLight into a coupled physical-biological model. We then compared predicted chlorophyll concentrations and nutrients for an idealized open-ocean simulation of mid-latitude Case 1 waters for approximate analytical vs. accurate numerical (EcoLight) irradiance calculations.

In these simulations, the predicted chlorophyll concentrations differed by a few tens of percent over the course of 10-year simulations owing to the differences in the approximate vs. accurate irradiances. This speaks well of the approximations used within the analytic light model for Case 1 water. More importantly, the EcoLight code runs with no more than a 30% increase in total run time, while providing several advantages than cannot be obtained with an analytic light model. These advantages are

- **EcoLight does a much better job of computing irradiances near 400 and beyond 00 nm, and at great depths.** These differences can have significant effects on how particular phytoplankton functional groups evolve in time and at depth.
- **EcoLight can model any water body, including Case 2 water and optically shallow waters** for which bottom reflectance can substantially increase the irradiance available for photosynthesis and water heating.
- **EcoLight provides the outputs necessary for ecosystem validation** using, for example, satellite-derived water-leaving radiances or remote-sensing reflectances, **without the necessity of using a chlorophyll algorithm** to convert satellite data into an ecosystem variable.
- **EcoLight provides a means for improved ecosystem model initialization and data assimilation directly in terms of the available data** (IOPs, irradiances, remote sensing reflectances), again **without an intermediate step involving a data-to-chlorophyll conversion algorithm.**
- **EcoLight costs at most 30% extra in the total simulation run time.** This is a small computational price to pay for its advantages.

2. Background

The fundamental measure of light energy in an aquatic system is the spectral radiance, which in horizontally homogeneous water bodies is a function of depth, direction, and wavelength. However, for ecosystem modeling the directional information contained in the radiance is usually irrelevant, because water constituents such as phytoplankton and dissolved substances are assumed equally likely to interact with light regardless of its direction of travel or state of polarization. Therefore, the spectral scalar irradiance as a function of depth z and wavelength ë, E_o(z,ë), is the fundamental radiometric quantity necessary for predictions of aquatic primary productivity, heating of water, and photochemical reactions. When modeling photosynthesis, which depends on the number of photons absorbed, it is necessary to multiply E_o(z,ë) by ë/hc, where h is Planck's constant and c is the speed of light. This converts the energy units of the spectral irradiance, W m^{-2} nm^{-1}, to quantum units, photons s^{-1} m^{-2} nm^{-1}.

A wavelength-integrated measure of the total light available for photosynthesis, the Photosynthetically Available Radiation (PAR), has historically been used in simple ecosystem models. Simple analytical models are commonly employed for estimating the dependence of PAR on time (diurnal to seasonal changes), depth, and water properties. These models are often parameterized by the chlorophyll concentration. Climatological data are often used to provide the time dependence of the (downwelling) surface irradiance. Traditionally, coupled ecosystem models have incorporated simple analytical formulas to predict $PAR(z)$ from a given chlorophyll profile and from an estimate of PAR at the sea surface. Although these analytical PAR models are computationally fast, they can produce estimates that differ by a factor of three near the sea surface and by a factor of ten at the bottom of the euphotic zone (Zielinski et al., 1998). Indeed, the depth of the euphotic zone, if defined as the depth where PAR decreases to one percent of its surface value, differs by almost a factor of two among these models. Errors of this magnitude are unacceptable for quantitative predictions of primary productivity or upper-ocean thermal structure. Additional inaccuracies can be found in the application of the PAR formulas, such as the use of downwelling plane irradiance E_d as a proxy for the scalar irradiance E_o.

Although simple PAR models are computationally convenient, any ecosystem model based on PAR is limited in its realism, regardless of how accurately PAR is computed. Different species of phytoplankton, or even the same species under different environmental conditions, have different pigment suites and thus respond differently to the same light field. Therefore, any biological model that attempts to describe competition between different species or functional groups having different pigments must use spectral irradiance, not a wavelength-integrated measure of the light.

The Ecosystem Simulation (EcoSim) model of Bissett et al. (1999a, 1999b) includes four phytoplankton functional groups, each with a characteristic pigment suite that changes over time with light and nutrient conditions. To model light effects on changes within and competition between these groups, EcoSim uses an approximate analytical model for the spectral scalar irradiance in Case 1 waters (described below). Although the EcoSim spectral irradiance model is sufficiently fast for use in coupled physical-biological ecosystem simulations involving many grid points and time steps, it does rest on several approximations that limit its accuracy even in Case 1 waters, and it is not applicable to optically shallow waters.

There is today much interest in the modeling of coastal waters, which are often Case 2 due to resuspended sediments or terrigenous particles and dissolved substances, and which may be shallow enough for bottom reflectance to make a significant contribution to the scalar irradiance. If EcoSim or similar models (e.g., Fujii, et al., 2007) are to accurately simulate such optically complex waters, they must incorporate spectral irradiance models that are computationally fast, accurate, and applicable to any water body or bottom condition. To address this need, I developed a specialized version of the HydroLight radiative transfer model, called EcoLight, which is designed to bring the optical component of ecosystem models up to the level of sophistication found in the latest physical and biological models.

3. Work Completed

The basic EcoLight code was developed with previous ONR funding and preliminary ecosystem simulations were made to show the importance and computational feasibility of accurate irradiance calculations. The current work incorporated EcoLight into a coupled physical-biological model and compared its performance with the analytical spectral irradiance model used in EcoSim. I first briefly describe the physical and biological models, and then EcoLight and the coupled model. I then compare the predictions made for an idealized ecosystem simulation when using the original EcoSim light model with those made using various EcoLight options.

The work reported here was performed in collaboration with Lydia Sundman of Sundman Consulting, Paul Bissett of the Florida Environmental Research Institute, and Bronwyn Cahill of Rutgers University, who were supported on this contract. All have contributed to this final report. This report is condensed from a draft journal article (Mobley et al., 2009), which is in preparation for submission to *Biogeosciences Discussions*.

3.1 The ROMS physical model

The physical model used here is a version of the Regional Ocean Modeling System (ROMS) described by Shchepetkin and McWilliams (2005; see also Fringer et al., 2006 and http://marine.rutgers.edu/po/index.php?model=roms). The ROMS model is a curvilinear-coordinate (terrain-following), free-surface, primitive equation model designed for prediction of physical oceanography quantities in coastal waters. The present study used a 6x6 horizontal grid version of ROMS 3.0 with periodic lateral boundary conditions. This spatially limited ROMS version was chosen to minimize run times during the EcoLight code development and verification simulations. For the simulations presented below, the grid is centered off the continental shelf of the eastern United States near 72.8 deg West and 38.8 deg North. The horizontal grid resolution is approximately 13 km. The vertical grid has 30 points covering the upper 202 m of the water column; the vertical resolution ranges from approximately 2 m near the sea surface to 15 m at depth.

3.2 The EcoSim biological model

The Ecosystem Simulation (EcoSim) biological model (Bissett et al., 1999a, 1999b) was developed for simulations of carbon cycling and biological productivity. This model includes four phytoplankton functional groups, defined according to their pigment suites (small diatoms, large diatoms, dinoflagellates, and *synechococcus*). Each functional group has a unique set of accessory pigments, which varies with the group carbon-to-chlorophyll *a* ratio, $C{:}Chl_a$. Pigment packaging and accessory pigment concentration are functions of the chlorophyll *a* concentration within each functional group. The chlorophyll *a* content and other properties of each functional group evolve with the light history and nutrient status of the group. The model also includes components describing dissolved and particulate organic and matter, bacteria, and detritus. The interactions between these components describe autotrophic growth of and competition between the four phytoplankton groups, differential (non-Redfield ratio) carbon and nitrogen cycling, nitrification, grazing, and air-sea exchange of CO_2. The initial application of EcoSim to predictions of seasonal cycles of carbon cycling and phytoplankton dynamics in the Sargasso Sea showed that its predictions were consistent with measurements of various biological and chemical quantities at the Bermuda Atlantic Time-series Study station (Bissett et al., 1999a).

An important component that was missing from the original EcoSim code was nutrient recycling. For the present simulations, subroutines were added to allow for vertical particle flux and restoration of nutrient fluxes that "fall through" the computational bottom back into the nutrient pool. Fecal material and phytoplankton now sink in EcoSim. When these hit the bottom, the flux of material from each component out of the system is converted directly into the appropriate nutrient and restored back into the nutrient pool. The result of this effort is that we can now obtain a nearly stable annual cycle over multi-year simulation periods.

The absorption spectra of the phytoplankton functional groups change with light and nutrient adaptation. The four groups therefore respond differently to various wavelengths of the available light, and each particular group responds differently over time. EcoSim requires spectral irradiances at 5 nm bandwidths between 400 and 700 nm in order to model the changes within each functional group and competition between them. The use of spectral irradiance rather than broadband PAR in modeling phytoplankton dynamics is a distinguishing feature of EcoSim.

EcoSim uses the RADTRAN atmospheric model (Gregg and Carder, 1990) to compute spectral downwelling plane irradiances just beneath the sea surface, $E_d(0,ë)$. These irradiances can be rescaled to match given irradiance values if the model is being driven by measured or climatological sky conditions. These subsurface spectral downwelling plane irradiances are then propagated to depth using

$$E_d(z,\lambda) = E_d(0,\lambda) \exp\left[-\int_0^z K_d(z',\lambda)\, dz' \right] \tag{1}$$

and a simple model for K_d,

$$K_d(z,\lambda) = \frac{a(z,\lambda) + b_b(z,\lambda)}{\bar{\mu}_d(z,\lambda)} . \tag{2}$$

Here a(z,ë) is the total absorption coefficient (the sum of absorption by pure water and the various particulate and dissolved components), and b_b(z,ë) is the total backscatter coefficient. The phytoplankton absorption is obtained from the concentrations of the functional groups and their chlorophyll-specific absorption spectra. The backscatter and total scatter coefficients are obtained from chlorophyll-dependent models for Case 1 waters, using the total chlorophyll-a concentration. The mean cosine for downwelling irradiance, ì $_{d}$(z,ë), is itself modeled by a simple function that merges estimates of the near-surface and asymptotic-depth mean cosines (Bissett et al., 1999b, Eqs. 18-22). Finally, the needed scalar irradiance E_o(z,ë) is obtained from the computed E_d(z,ë) via the approximation E_o(z,ë) = E_d(z,ë)K_d(z,ë)/a(z,ë).

The biology is updated at each time step and grid point using the analytic formulas for the scalar irradiance just described. However, the irradiances computed within EcoSim do not feed back to the ROMS code which, for programming simplicity when merging the codes, retains its original short and long-wave light parameterization for mixed-layer heating calculations. Thus the physical model influences the biology via temperature and mixing, but the optical model employed within EcoSim does not influence the physical model. This simplification was made in the present study to avoid alterations to the ROMS code.

3.3 The Ecolight irradiance model

Numerical models that solve the exact radiative transfer equation (RTE) are currently available (Mobley, et al., 1993) and can provide highly accurate predictions of the light field, in particular the scalar irradiance as a function of depth and wavelength. However, the computational times required by these exact numerical models are far too great for their inclusion in large coupled models that need irradiance predictions at many spatial locations and times of day during multi-year ecosystem simulations.

The HydroLight radiative transfer model (Mobley, et al., 1993; Mobley, 1994; www.hydrolight.info) provides an accurate solution of the unpolarized RTE for any water body, given the inherent optical properties (IOPs, namely the absorption and scattering properties) of the water body, the incident sky radiance, and the bottom reflectance (in finite-depth waters). Although the standard version of Hydrolight is computationally very efficient for predicting full radiance distributions, its run times are still much too long for use in ecosystem models.

I therefore developed a highly optimized version of Hydrolight 4.2, called EcoLight, which computes irradiances as a function of depth and wavelength for any water body, with the same accuracy as HydroLight. Related quantities such as the irradiance reflectance, nadir-viewing remote-sensing reflectance, diffuse attenuation functions, and mean cosines are also computed by EcoLight. Although those ancillary quantities are not needed as inputs to most ecosystem models, they can be of use in ecosystem model validation and data assimilation. Quantities such as the remote-sensing reflectance are not available from any of the simple analytic light models.

Ecosystem models require only the scalar irradiance as a function of depth and wavelength, which is computed from an azimuthal integration of the radiance. This means that the RTE can be azimuthally averaged to obtain an equation for the azimuthally averaged radiance as a function of polar angle. The numerical solution of the resulting RTE is much faster than in HydroLight. Various other simplifications to the EcoLight code were made. The most important are the use of a piecewise homogeneous water column, solution of the RTE to different depths at different wavelengths, and wavelength skipping.

The ROMS-EcoSim code models the water column as a stack of homogeneous layers of variable thickness. Therefore the IOPs within a given water layer are independent of depth. The EcoLight code takes advantage of the depth independence of the IOPs within a layer to reduce the computation needed to solve the RTE for the depth dependence of the irradiances within each layer.

HydroLight solves the RTE to a user-specified geometric depth, which is the same for every wavelength and must be chosen before the run is started. This becomes computationally expensive at wavelengths where the IOPs are large (e.g., due to water absorption at red wavelengths), corresponding to a large optical depth for a given geometric depth. EcoSim requires the spectral scalar irradiance only to the bottom of the euphotic zone, below which it does not perform primary production calculations. Therefore, it is necessary to compute the irradiance only to that depth, which varies with the biological state of the ocean and cannot be predetermined.

In EcoLight the goal is to solve the RTE to the shallowest depth possible and then to extrapolate the scalar irradiance to greater depths. To determine the depth to which the RTE is to be solved at a particular wavelength, an estimate is first made of the depth z_o to which the scalar irradiance at the current wavelength will decrease to a factor F_o of the surface value (e.g., $F_o = 0.1$, corresponding to the 10% light level). The RTE is then solved exactly to depth z_o. The computed scalar irradiance $E_o(z_o$,ë) is then objectively extrapolated to all depths below z_o using a variant of Eq. (1), namely

$$E_o(z,\lambda) \;=\; E_o(z_o,\lambda)\exp\left[-\int_{z_o}^{z} a(z',\lambda)\,dz'\right]. \tag{3}$$

HydroLight numerical simulations show that the scalar irradiance varies with depth in correlation with the depth variation of the total absorption coefficient $a(z'$,ë), once z_o is below the depth at which surface boundary effects are important. This is to be expected because K_d in Eq. (1) is a very "absorption-like" parameter, and K_o is close to K_d away from the sea surface (becoming equal to K_d at great depths).

There is also an EcoLight option to solve the RTE at only some wavelengths, and to obtain the irradiances at the unsolved wavelengths by interpolation. For example, EcoLight can solve the RTE at every n^{th} EcoSim wavelength (n = 2, 3, ...) and then estimate the irradiances at the unsolved wavelengths by interpolation between the computed wavelengths. Solving the RTE only at every n^{th} wavelength gives a factor of n decrease in the EcoLight run time, all else being equal.

In summary, EcoLight takes the following philosophy. It is necessary to solve the RTE in order to incorporate the effects of the surface boundary conditions and to account for all IOP effects. However, once an accurate value of $E_o(z_o$,ë) has been computed to some depth z_o deep enough to be free of surface boundary effects, it is not necessary to continue solving the RTE to greater depths, which is computationally expensive. As shown in Section 4, it is possible to extrapolate the accurately computed upper-water-column irradiances to greater depths and still obtain irradiances that are acceptably accurate for ecosystem predictions. Likewise, as shown below, it is not necessary to solve the RTE at every EcoSim wavelength in order to obtain acceptably accurate irradiances at the needed wavelength resolution.

3.4 The ROMS-EcoSim-EcoLight coupled model

The ROMS and EcoSim models were previously coupled by P. Bissett, and that code served as the starting point for the nutrient recycling modifications and the incorporation of EcoLight. The analytic irradiance model used in the standard EcoSim code was replaced by a call to the EcoLight subroutine. EcoSim passes EcoLight the current total IOPs as functions of depth and wavelength, atmospheric conditions (as needed by RADTRAN, which is also used by EcoLight to compute the spectral irradiance incident onto the sea surface), wind speed, grid depths, and other information needed by EcoLight. After solving the RTE, EcoLight returns the scalar irradiance $E_o(z$,ë) to EcoSim for use in its primary production calculations. The diffuse attenuation function K_d, mean cosine ì $_d$, remote-sensing reflectance, downwelling plane irradiance E_d, and various other quantities are also returned to EcoSim. Although these quantities are not needed for EcoSim's biological computations when EcoLight is used, they are of interest for comparison with the analytic values and for model validation when comparing ecosystem predictions with actual measurements. These quantities are saved to files for post-run analysis. In the current code, the EcoLight-computed irradiances are used only within EcoSim; ROMS still uses its original irradiance model for its thermodynamics calculations. Although the ROMS parameterization of solar transmission into the water column is oversimplified (Paulson and Simpson, 1977; Cahill et al., 2008), it was retained here to avoid modifications to the ROMS code itself.

4. Results

4.1 Simulations

The ROMS-EcoSim and ROMS-EcoSim-EcoLight models were run in various modes for ten-year simulations to determine the differences in ecosystem evolution owing to differences in the irradiance calculations, all else (ecosystem structure, vertical mixing, external forcing) being held the same.

As noted in §3.1, the 6x6 ROMS grid used here was located off the east coast of the U.S. The corresponding external forcing for solar irradiance and surface wind speed as used in ROMS was obtained from a one-year time series of measured values from ECMWF 40-year reanalysis of gridded atmospheric data at six-hour resolution. We used both daily averages and hourly values derived from these data in our simulations. The RADTRAN clear-sky irradiance computations used within EcoSim were driven the latitude, longitude, and time of day, and the RADTRAN clear-sky spectral irradiances were rescaled to match the measured wavelength-integrated values used by ROMS. The ROMS-computed circulation and mixing are identical in all runs because the irradiances computed and used within EcoSim for its biological calculations are not passed back to ROMS for its water-heating calculations. The differences in the predicted ecosystem evolution are thus due to differences in the irradiances computed within EcoSim, either by its default analytic model or by EcoLight, and used there for its primary production calculations.

Given the geographical location of the ROMS grid, its periodic lateral boundary conditions, and the external forcing, the present simulations can be thought of as modeling idealized mid-latitude, open-ocean, Case 1 water. We did not attempt here to model any specific ecosystem, which would require a fully 3D spatial grid tailored to the boundary conditions of the location being modeled.

This annual cycle of external forcing was repeated for each year of the simulation. The long-term annual cycle of the ecosystem variables should thus depend only on the ecosystem structure, i.e., on the form of the interactions between the biological functional components, on the nature of the vertical mixing used in the physical model, and on the values of parameters that describe strengths of various interactions. The assumed ecosystem initial conditions and numerical transients should affect only some initial time period of a simulation, after which the ecosystem should reproduce an annual cycle that is independent of the initial conditions.

4.2 Model initial conditions

The coupled ROMS-EcoSim model with its analytical light calculations was first run to examine its behavior over long simulation times. To test the independence of the final ecosystem state from the initial conditions, this model was run with baseline initial (at time 0) concentration vs. depth profiles for the biological functional groups. The baseline initial concentrations for the four phytoplankton functional groups are shown in Fig. 1. Those concentrations were then halved and doubled to obtain other sets of initial conditions. Figure 2 shows the results for the total chlorophyll concentration at a depth of 1 m for the first year of the simulations. Halving and doubling the initial concentrations affects the predicted total chlorophyll values for only the first few months of a simulation. Larger perturbations in the initial conditions require longer to converge, but the predictions do approach the same annual cycle in later years. The ecosystem final state is thus independent of the initial conditions of a simulation, as expected.

4.3 Ecosystem simulations

The ROMS-EcoSim model with its baseline initial conditions and its analytic light (AL) model was run in its standard mode for a 10-year simulation to generate the baseline ecosystem prediction for comparison with various runs using the EcoLight (EL) irradiance calculations. In this AL run, the irradiances were computed at every grid point (denoted in the figure as EGP), every ROMS time step (ETS), every wavelength (5 nm), and down to the $F_o = 0.001$ (0.1%) light level. Figure 3 shows the resulting surface total chlorophyll values over the 10 years (the red curve). This run required 5.28 hours on an Apple iMac with a 2.16 GHz processor and 1 Gbyte of RAM., or about 32 minutes per simulation year.

The analytic light model in ROMS-EcoSim was then replace by calls to EcoLight, which was run in various modes for comparison with the AL baseline run. When EcoLight is called at every grid point, every time step, 5 nm, and the RTE is solved down to the $F_o = 0.001$ light level, the run times are prohibitively long (estimated to be 400 hours for a full 10-year simulation). However, the EcoLight chlorophyll predictions are essentially the same (to within 1% at all times over simulations of a year) when EcoLight is called at only 1 grid point (1GP). The irradiances at the other grid points are then obtained by scaling the $E_o(z,\text{ë})$ values at the computed grid point by the incident sky irradiance at the other grid points. This reduces the run time for a 10-year simulation to 85.7 hours. This EL, 1GP, ETS, 5 nm, $F_o = 0.001$ simulation is taken to be the baseline EcoLight run for comparison with the 10-year AL run and with other EL runs. The resulting surface chlorophyll values are shown in green in Fig. 3.

After an initial period of numerical and biological adjustment to the initial conditions, both light models show a long-term trend of slowly decreasing chlorophyll values from one year to the next, with annual-average chlorophyll values (dotted lines in Fig. 3) decreasing by about 6% a year. This is likely due to inadequate vertical mixing to replenish the nutrients from deep water below the maximum depth of the simulation, which was 202 m. It should be remembered that these simulations are for a small spatial grid that cannot reproduce lateral advection as occurs in a true 3D ecosystem, and that we are using a specific parameter setup for the phytoplankton populations. While undesirable, this trend does not affect our comparison of the differences in ecosystem behavior due to different light calculations, with all else being the same.

Even though the differences are not great, we believe that this baseline EL simulation better represents the evolution of the modeled ecosystem because the EcoLight irradiances are accurately computed throughout the water column at all wavelengths, rather than being obtained from the overly simple approximate analytical model of the AL simulation. In particular, it must be remembered that the phytoplankton functional groups in EcoSim each have their own photosynthetic action spectra, so that they utilize different wavelengths in different ways, and thus respond differently to the spectral composition of the scalar irradiance $E_o(z,ë)$. EcoLight does a better job of modeling $E_o(z,ë)$ near 400 nm, beyond 600 nm, and at depth (Fig. 7, discussed below). These differences may have important ecological impacts for some functional groups.

The baseline EL simulation run time is still far too long for routine ecosystem simulations. However, it is not necessary to recompute the irradiances at every ROMS time step. In the next run, EL was called at 1 grid point and the in-water irradiance was recomputed only every 4 hours (4HR), rather than at every ROMS time step. The most recently computed irradiance was then re-scaled by the input sky irradiance at the current time, and the resulting irradiance profile was used. The irradiances were computed at 25 nm resolution and interpolated to the 5 nm resolution required by EcoSim. Finally, the RTE being solved down to only the 15% (F_o = 0.15) light level and extrapolated to the 0.1% level needed by EcoSim using Eq. (3). With these optimizations, the total EL run time was reduced to 6.88 hours. The resulting ecosystem predictions remain the same as for the baseline EL simulation to within 5% at all times, and are usually closer. This is an increase of only 30% in total run time over the AL simulation, but preserves the ecosystem behavior of the high-resolution EL simulation. ***This is a small increase in total computation time compared to the advantages of using an accurate light model that gives a wide range of output needed for ecosystem validation or for initialization and data assimilation.***

Figure 4 shows year ten of the simulation. The AL and EL baseline runs are the same as seen in year 10 of Fig. 3. The blue curve shows the optimized EL simulation just described: 1GP, 4HR, 25 nm, F_o = 0.15.

Another run was made with EcoLight further optimized to 1GP, 6HR, 50 nm, and Fo = 0.5. The resulting run time decreased to 6.73 hours. However, this optimization proved to be too coarse of a computational scheme in that the resulting ecosystem behavior differed significantly from the EL base. The surface chlorophyll values differed by as much as 32% (with greater differences at depth), and the time of the spring bloom was approximately a month late. These results are thus deemed to be unacceptable. This curve is shown in violet in Fig. 4.

Figure 4 reveals surprisingly small differences between the long-term AL and EL annual cycles (omitting the over-optimized violet EL curve from further consideration). The maximum daily near-surface chlorophyll difference is about 23%, with EL being greater than AL. The annual averages are 2.65 mg m^{-1} for EL and 2.42 mg m^{-1} for AL, or about a 10% difference. The times of the spring bloom are about the same in both models. We view this good agreement as a welcome test of the accuracy of the EcoSim analytic light model for Case 1 water and as a model-model validation of the correct implementation of both codes for computing in-water irradiances.

Similar results are found at greater depths, although the differences can be somewhat greater. Figure 5 shows the year 10 total chlorophyll values at depth 15.7 m. At this depth, the maximum difference between AL and EL is 36%, although the annual averages are within 4% of the same. Figure 6 shows the depth profiles of total chlorophyll at day 180o8 of year 10, when the water column was well stratified in mid-summer.

The run parameters and the run times for these simulations are summarized in Table 1. Table 2 shows the percent of total run time used for the physical (ROMS) vs. bio-optical (EcoSim with or without EcoLight) components of the ecosystem numerical model.

model	**time resolution**	**grid resolution**	F_o	**wavelength resolution**	**run time in hours**
Analytic	9 min (every ROMS time step)	every grid point	0.001	5 nm	5.28
EcoLight (run 1 year)	9 min	every grid point	0.001	5 nm	est. 400
EcoLight	9 min	1 grid point	0.001	5 nm	87.5
EcoLight	every 4 hours	1 grid point	0.15	25 nm	6.88
EcoLight	every 6 hours	1 grid point	0.5	50 nm	6.73

Table 1. Options used in comparison runs. The run times are on a 2.1 GHz Mac for 10-year simulations. The last EcoLight option gave unsatisfactory results.

simulation	**physical module**	**bio-optical module**
AL base run	60.2	39.8
EL base run	3.7	96.3
EL optimized run A	46.2	53.8

Table 2. Percent of total run time for 10 year simulations used by the physical and bio-optical modules of the coupled ecosystem model.

4.4 Irradiance comparisons

We next consider how the analytic and numerical light models compare in their computed irradiance values. The answer can be seen by comparison of the spectral plane irradiances E_d(z,ë) at time 0 of the simulation, when the water column inherent optical properties are identical in all models. Figure 7 shows the initial E_d(z,ë) computed by the AL and the two EL models used in Figs. 4-6. The irradiances for these three models are close throughout the euphotic zone, in the green part of the spectrum. However, the analytic-model irradiances are less the EcoLight's irradiances near

400 nm and at red wavelengths, with the differences becoming orders of magnitude at depth. The two EcoLight versions are fairly close to each other at all depths and wavelengths, although some differences due to wavelength interpolation and depth extrapolation are apparent, as expected.

The reason for the differences in the analytic and EcoLight spectral scalar irradiances can be traced to the differences in the mean cosine ì$_d$ and diffuse attenuation K_d for the three models. A comparison at only one wavelength, 442 nm, will suffice. Figure 8 shows the ì$_d$(442) depth profiles at time 0. The analytical model for ì$_d$(442) is much different than the mean cosines computed by EcoLight. In particular, the analytical ì$_d$(442) approaches 0.5 at large depths, implying an isotropic downwelling plane irradiance, which is not correct for any ocean waters. Even at asymptotic depths in homogenous water, the radiance distribution is far from isotropic and typical ì$_d$(442) values are around 0.7 to 0.8 at great depth, as seen in the figure for EL runA. Note that EL runB solved the RTE only to the 15% light level, which was about 10 m at this time and wavelength. Forcing ì$_d$ = 0.5 at great depth is an easily correctable weakness of the default analytic mean cosine model used in EcoSim. Note that in the full EcoLight calculation, the mean cosine continues to increase slowly with increasing depth.

In the analytic irradiance model, the mean cosine is used to determine the K_d depth profile as seen in Eq. (2). In the present simulation, ì$_d$(442) is too small and K_d(442) is consequently too large, as seen in Fig. 9. The too-large K_d then makes E_d, and consequently E_o, too small, as seen in Fig. 7. These analytic vs. EcoLight differences in E_o(z,ë) at time 0 then lead to slightly different biological concentrations at the second time step. These differences then lead greater differences in ecosystem chlorophyll values as time goes on.

5. Conclusions

Figures 3-9 and Tables 1 and 2 are sufficient to establish the primary results of this study. In spite of this relatively good agreement for this particular idealized simulation of deep Case 1 water, we argue for the future use of EcoLight for the following reasons:

- **EcoLight does a much better job of computing irradiances near 400 and beyond 600 nm, and at great depths.** These differences can have significant effects on how particular phytoplankton functional groups evolve in time and at depth.
- **EcoLight can model any water body, including Case 2 water and optically shallow waters** for which bottom reflectance can substantially increase the irradiance available for photosynthesis and water heating.
- **EcoLight provides the outputs necessary for ecosystem validation** using, for example, satellite-derived water-leaving radiances or remote-sensing reflectances, **without the necessity of using a chlorophyll algorithm** to convert satellite data into an ecosystem variable.
- **EcoLight provides a means for improved ecosystem model initialization and data assimilation directly in terms of the available data** (IOPs, irradiances, remote sensing

reflectances), again **without an intermediate step involving a data-to-chlorophyll conversion algorithm.**

- **EcoLight costs at most 30% extra in the total simulation run time.** This is a small computational price to pay for its advantages.

Although simple analytic irradiance models do run extremely fast, there is little justification for their use in light of their potential inaccuracies and inconsistencies, even for Case 1 waters. Moreover, some analytic models (although not EcoSim) parameterize the water inherent optical properties in terms of a single quantity—the total chlorophyll concentration—which greatly oversimplifies the complex relation between light propagation and the scattering and absorption properties of various ocean constituents. Sophisticated ecosystem models such as EcoSim therefore track several functional groups of particles, each of which has its own absorption and scattering properties. EcoSim determines its total inherent optical properties as sums of the contributions by any number and type of components and is thus able to model changes in the light field induced by changes in the concentration or optical properties of whatever functional groups are included in the biological model. Such connections between ecosystem components and the light field cannot be simulated by simple analytic models.

Computational stability criteria for ecosystem physical models may require time steps as small as one minute. However, as shown here, it is not necessary to update the light field at each time step. It is adequate to run Ecolight at longer intervals and then interpolate to the desired time. The same idea applies to running Ecolight on a coarser spatial grid than the ecosystem model uses and then interpolate to obtain the required spatial resolution. In practice, in fully 3D simulations, it would probably be possible to dynamically determine when to call EcoLight. For example, as the calculations proceed to a new grid point, the IOPs at that grid point could be compared with those at the last grid point where EcoLight was called (the reference point). If the IOPs at the new grid point differ by less than some amount from those at the reference point, then the previously computed irradiances would be rescaled, as was done with the 1GP calculations studied here, and applied at the new grid point. If the IOPs at the new grid point differ by more than some amount from those at the reference point, then EcoLight would be called for a *de novo* calculation of the irradiance, and the current grid point would become the new reference point. A dynamic determination of when to call EcoLight would allow for frequent calls near fronts or in other situations where the IOPs or external properties are changing rapidly, and for few calls in fairly homogenous and stable ocean regions. When employed is this manner, Ecolight should be applicable to three-dimensional ecosystem models requiring spectral irradiances at many wavelengths and on a fine spatial and temporal grid, but at little more computational expense than the default analytical light model being applied at every time step and grid point, as is done now.

6. Scientific Impact

Light is an important factor in determining primary production and mixed-layer dynamics, so EcoLight's accurately computed spectral scalar irradiances will significantly improve ecosystem model predictions, compared to the use of approximate analytical models for spectral irradiance or PAR. Moreover, predictions of primary production in shallow waters and for seagrass beds, for which analytic chlorophyll-based models can be off by a factor of ten or more near highly reflecting substrates, would be well-served by the use of Ecolight.

In addition, EcoLight computes the water-leaving radiance and nadir-viewing remote sensing reflectance at no extra cost. This allows for direct ecosystem model validation using satellite-derived remote-sensing reflectances, without the use of a chlorophyll algorithm to convert the satellite remote-sensing reflectance to a chlorophyll value for comparison withe the predicted chlorophyll value. Such chlorophyll algorithms are inaccurate even in open-ocean, Case 1 waters, and they can be in error by over an order of magnitude in coastal, Case 2 water. They are not applicable at all in shallow water for which bottom reflectance influences the water-leaving radiance.

Finally, EcoLight computes other standard optical quantities of interest such as various in-water irradiances, reflectances, and diffuse attenuation functions. These quantities can also be of use for ecosystem validation and, importantly, for model initialization and for data assimilation when data on these variables are available from observation or ancillary models.

7. Future Work

We have properly incorporated EcoLight as a subroutine into EcoSim in the sense that EcoLight is getting the correct IOPs and other information from ROMS and EcoSim, solving the RTE correctly, and returning accurate irradiances to EcoSim for use there. However, we have made no attempt to rewrite the EcoLight code to bring it up to ROMS-EcoSim standards, which would be necessary for efficient simulations on large spatial scales over years of time. The EcoLight code, which is called as a subroutine from EcoSim, remains mostly Fortran 77 and contains many features that are not really needed for ecosystem simulations. We speculate that a thorough rewriting of EcoLight in Fortran 95 and removal of unneeded features might gain another factor of two in run times. Use of a faster ODE solver for depth integration of the RTE, which is where most of EcoLight's run time is used, should also be investigated.

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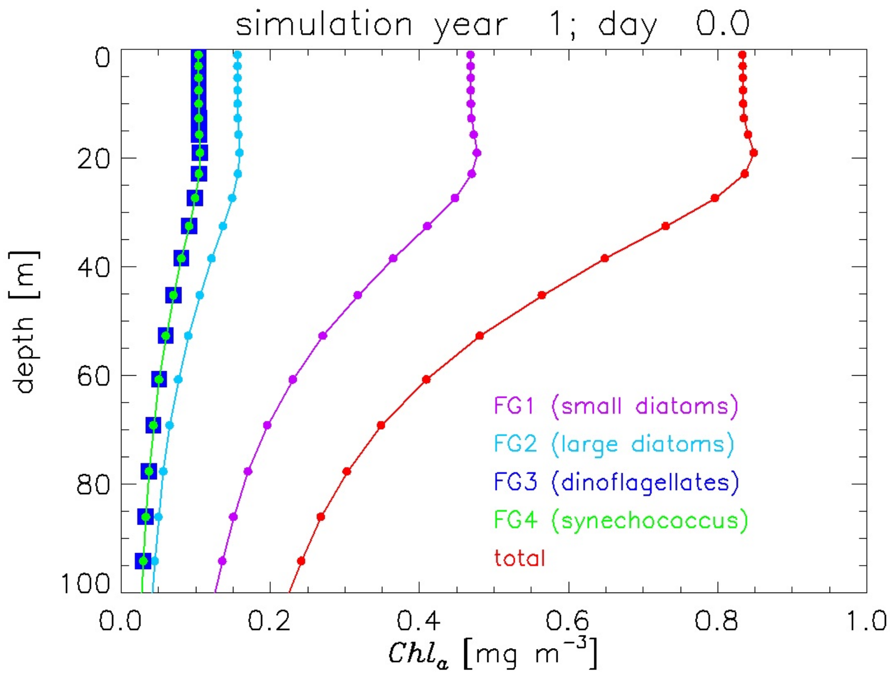

Fig. 1. Initial depth profiles of the chlorophyll concentrations of the four phytoplankton functional groups, and of the total chlorophyll.

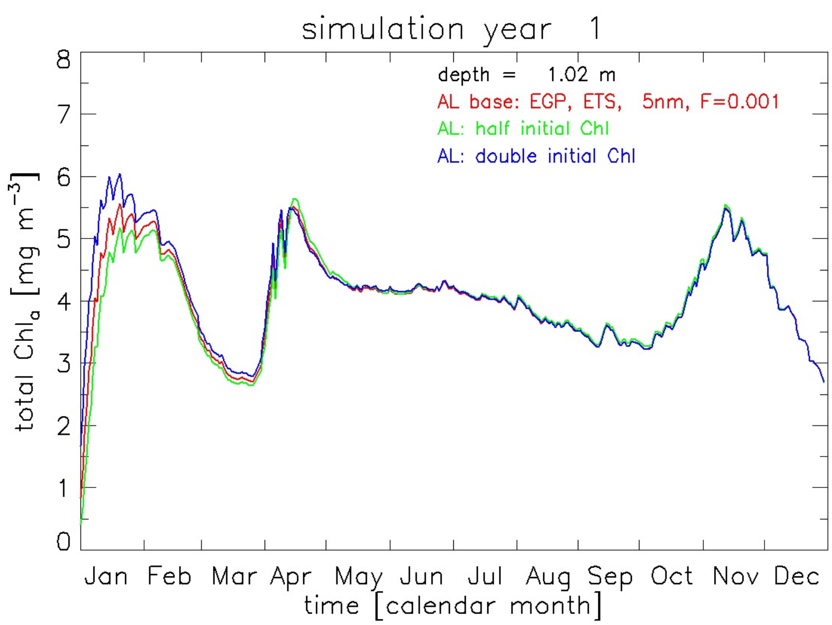

Fig. 2. Time series during year 1 of total chlorophyll at 1 m depth for the analytic light model and 3 sets of initial conditions. The base conditions (red curve) at time 0 are those seen in Fig. 1.

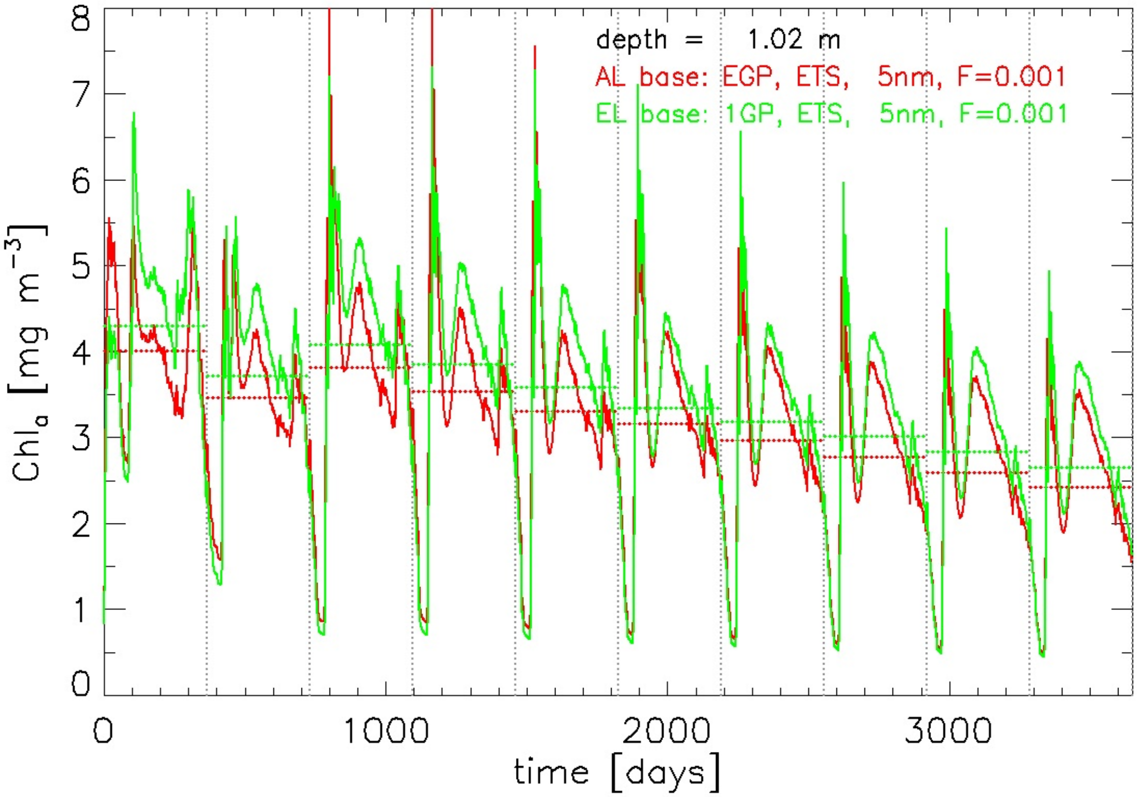

Fig. 3. Ten-year simulations for the baseline analytic (AL, red) and EcoLight (EL, green) simulations. The predicted total chlorophyll values are plotted at local noon of each day. The annual average Chl values are shown by the horizontal dotted lines within each year.

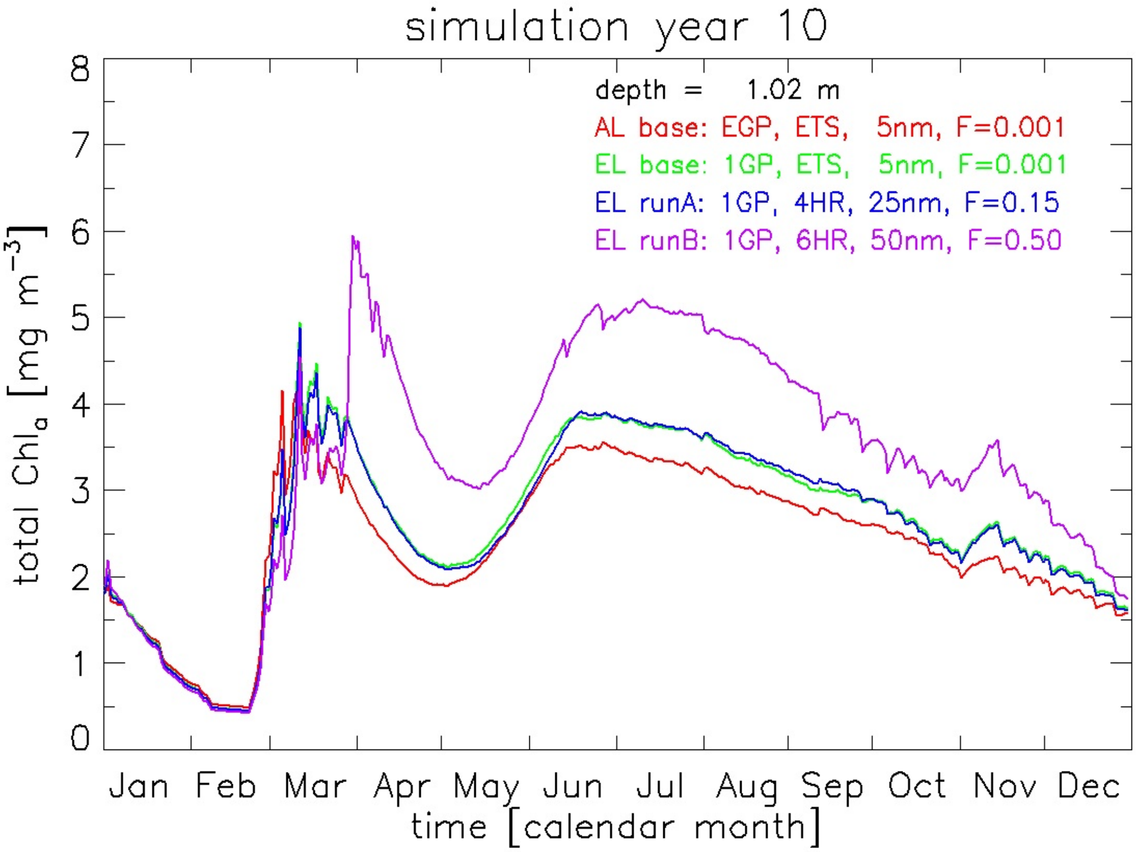

Fig. 4. Total chlorophyll values at 1 m depth during year 10 of the simulation. The irradiance calculation models are identified on the inset labels.

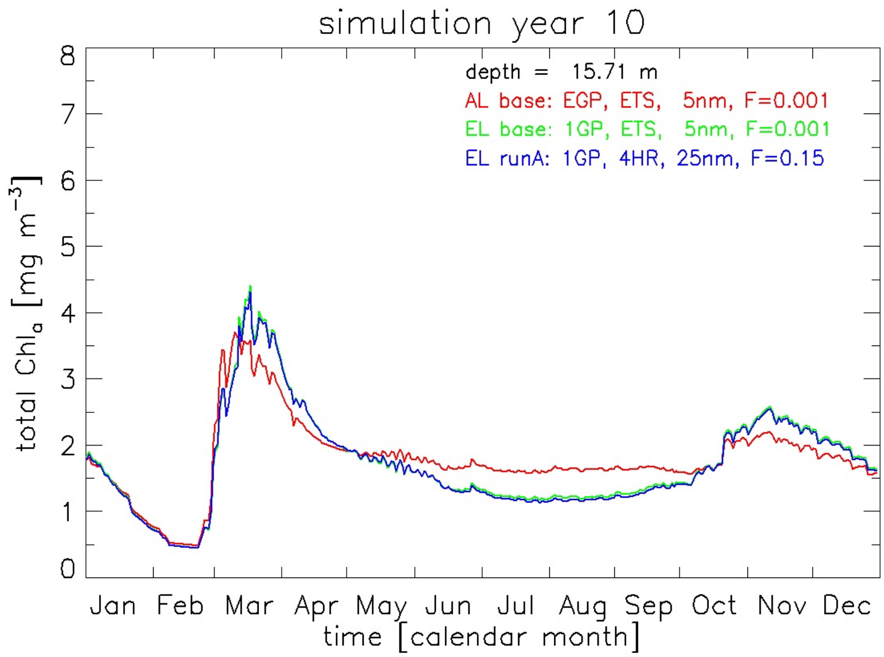

Fig. 5. Chlorophyll concentrations during year 10 at depth of 15.7 m for various simulations.

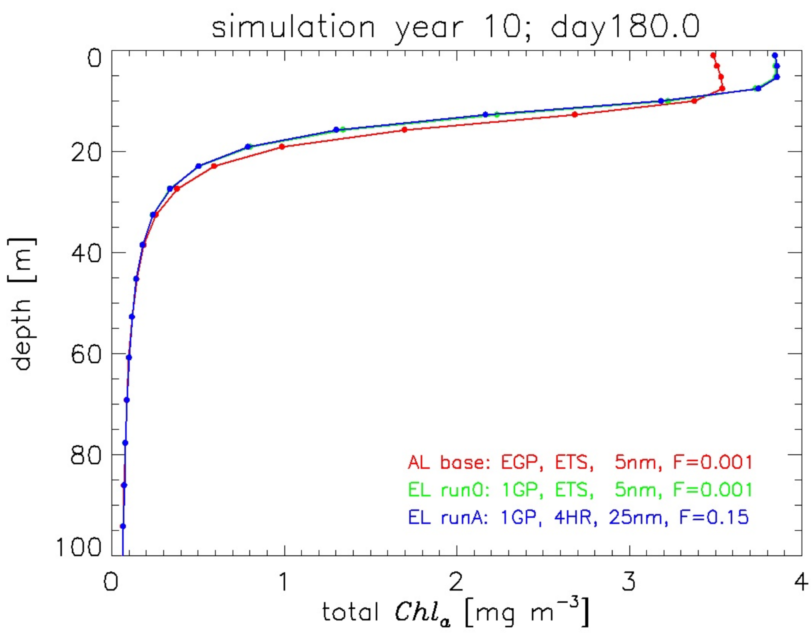

Fig. 6. Chlorophyll concentrations at as a function of depth at day 180 of year 10.

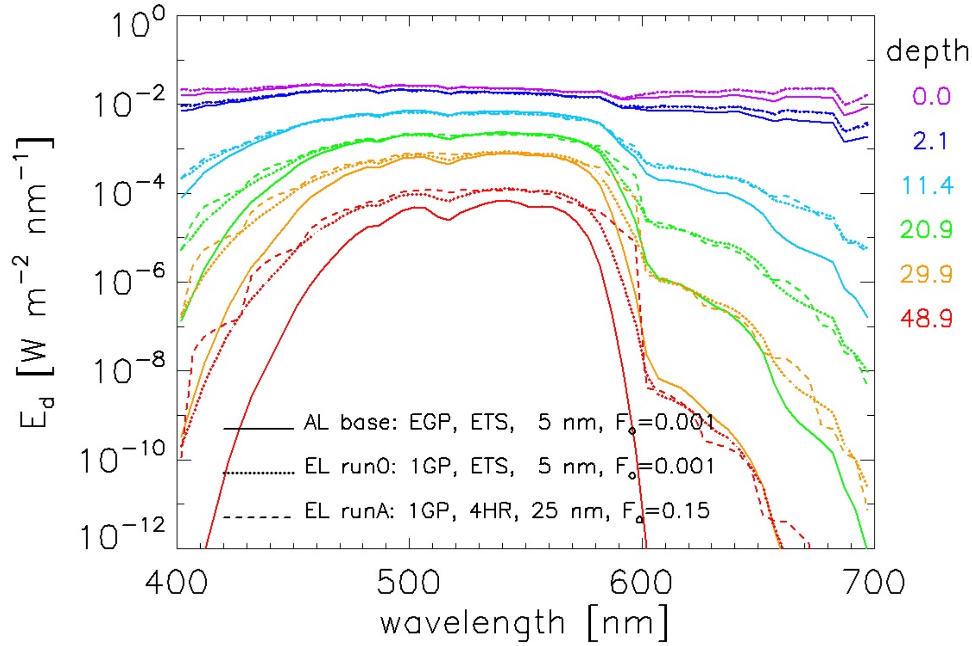

Fig. 7. The spectral downwelling plane irradiances E_d at time 0 at selected depths.

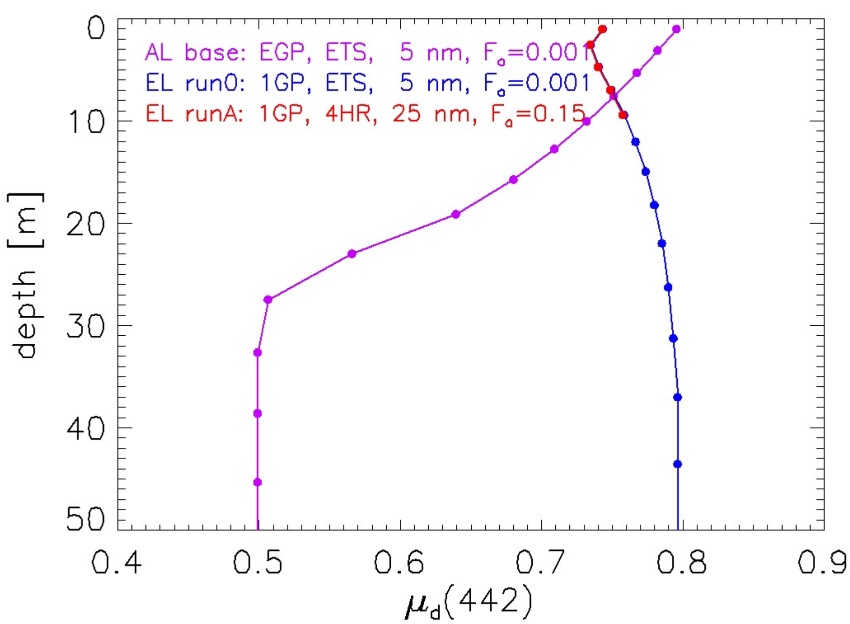

Fig. 8. The mean cosine for downwelling radiance at 442 nm, ì $_d$(442), at time 0. Run A solved the RTE down to only 10 m at this wavelength.

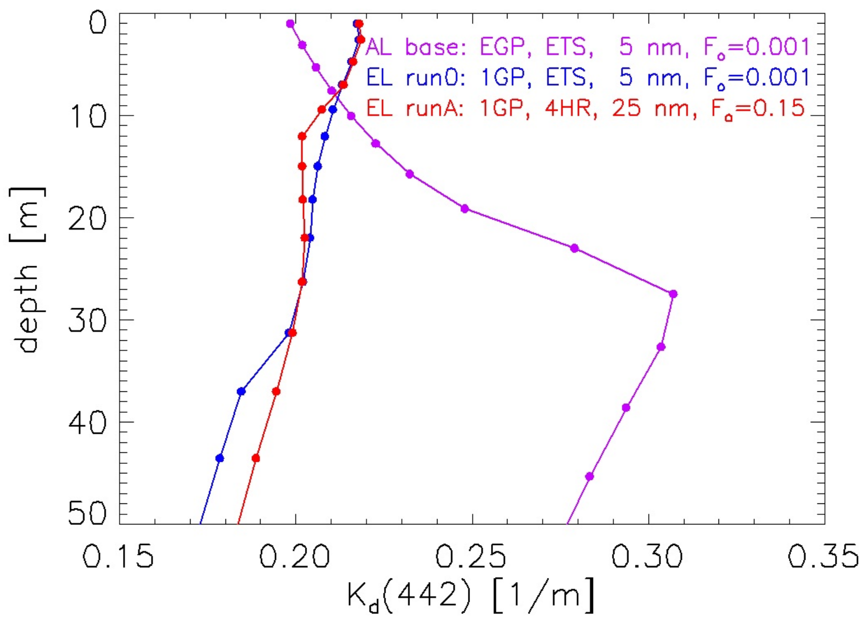

Fig. 9. The diffuse attenuation coefficient for downwelling plane irradiance at 442 nm, $K_d(442)$, at time 0. The Run A values are from the extrapolation to depth by Eq. (3), rather than from solving the RTE.